CFD INVESTIGATION ON HYDROGEN ENRICHMENT EFFECT TO DUAL-FUEL DIRECT INJECTION DIESEL ENGINE

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A thesis submitted in
fulfilment of the requirement for the award of the
Doctor of Philosophy

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FEBRUARY 2021

I hereby declare that the work in this thesis is my own except for quotations and summaries which have been duly acknowledged

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DEDICATION

To the memory of my mother and father, who would have being glad to see me at this moment.

To my wife and beloved children, Reime, Yeser, Fadel and Huda for their love and support.

To my brothers and sisters for their support and encouragement

To all my family members and friends for their love and support

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ABSTRACT

The engine as an integral and most important part of the vehicle which the mechanical power used in moving the automobile. Compression Ignition (CI) engines are use in driving heavy duty machines and power generation plants due to the 40% higher efficiency and torque compared to the Spark Ignition (SI) engines. Bulk of previous studies on the use of alternative fuels; hydrogen-natural gas blends (HCNG) used port injection and experimentally were conducted. The use of Computational Fluid Dynamics (CFD) simulations in analyzing the effect of adding (0 - 90) % hydrogen to blend fuel and varying the equivalence ratio (0.6-1.4) on the combustion and exhaust emission characteristics are not intensively studied. Especially when using direct injection (DI) technique. The aim of this study was to develop a reliable CFD model capable of predicting the key parameters in the combustion process of a DI-diesel engine. The study investigated the relationship between hydrogen and variations in equivalence ratio on the air-fuel dynamic flow and emissions characteristics. The simulation using HCNG was conducted at various hydrogen doses (0 – 90) % along equivalence ratios of 0.6 -1.4 at a step of 0.2. The constant engine speed was 1500 rpm at low load condition. The developed CFD model was validated for reliability using a comparative analysis with other experimental study. The result of validation showed that the CFD model was in close agreement with the experimental work used in confirmation. The addition of 0% - 90% hydrogen increased the in-cylinder temperature from 1017 K at 0% to 1200 K at 90 %, when the equivalence ratio was 0.6. At 90 % added hydrogen, the maximum in-cylinder temperature of 1424 K was obtained. A reduction in the in-cylinder pressure from 3.200 bar at 0% hydrogen to 2.872 bar was obtained at 90 %. Increase in equivalence ratio increased pressure to 3.228 bar at 1.4 equivalence ratio and 0 % hydrogen. Heat release rate (HRR) increased when both mole fraction of hydrogen and equivalence ratio increased, with 37.98 KJ as the maximum heat release rate observed at 90 % hydrogen addition and 1.4 equivalence ratio. CO increased with hydrogen and decreased with increase in equivalence ratio. At 90 % hydrogen (0.6 equivalence ratio), the maximum CO of

0.0306 mole fraction was obtained, while the minimum of 0.0201 mole fraction was obtained at 1.4 equivalence ratio. On the contrary, the emission of CO_2 mole fraction decreased with increase in hydrogen mole fraction and increased with increase in equivalence ratio. NO_xemission increased with increase in both parameters. The mole fraction of unburnt methane increased with mole fraction of hydrogen and decreased with increase in equivalence ratio. Swirl ratio decreased with decrease in both parameters, whereas tumble ratio increased with increase in both parameters respectively. The contour analysis of the effect of addition of hydrogen on the heat flux losses showed that the bulk of flame contour expanded around the piston bowl with increase in the mole fraction of hydrogen. Addition of hydrogen increased the tumble ratio. The maximum range of velocity was 9.72-8.26 m/s and 6.80-5.35 m/s within the piston bowl region. The results show that, increasing hydrogen in natural gas-diesel improved the combustion characteristics and reduced emissions in the CI engine.

ABSTRAK

Enjin sebagai bahagian paling utama dan terpenting bagi sesebuah kenderaan yang menggunakan tenaga mekanikal untuk menggerakkan automobil. Enjin jenis Pencucuhan Mampatan (CI) telah digunakan dalam menggerakkan mesin tugas berat dan janakuasa penjanaan tenaga kerana kecekapan dan torknya yang 40% lebih tinggi berbanding dengan enjin Pencucuhan Bunga Api (SI). Sebilangan besar kajian terdahulu mengenai penggunaan bahan bakar alternatif; contohnya campuran gas hidrogen asli (HCNG) menggunakan suntikan liang (port injection), dan telah dijalankan secara eksperimental. Penggunaan simulasi Perkomputeran Dinamik Bendalir (CFD) dalam menganalisis kesan penambahan (0 - 90) % hidrogen pada adunan bahan bakar dan mengubah nisbah kesetaraan (0.6-1.4) pada ciri pembakaran enjin dan pelepasan ekzos tidak pernah dikaji secara intensif. Terutama semasa menggunakan teknik suntikan langsung (DI). Tujuan kajian ini adalah untuk membangunkan model CFD yang boleh dipercayai, yang berupaya meramalkan parameter utama dalam proses pembakaran enjin DI-diesel. Kajian ini menyelidiki hubungan antara hidrogen dan variasi dalam nisbah kesetaraan ke atas ciri aliran dinamik udara bahan api dan pelepasan. Simulasi menggunakan HCNG telah dijalankan pada pelbagai dos hidrogen (0 - 90) % di samping nisbah kesetaraan 0.6 - 1.4 pada setiap langkah 0.2. Kelajuan enjin ditetapkan ialah 1500 rpm pada kondisi bebanan rendah. Model CFD yang dibangunkan telah disahkan kebolehpercayaannya dengan menggunakan analisis komparatif dengan kajian eksperimental yang lain. Keputusan pengesahan menunjukkan bahawa model CFD memberikan dapatan yang hampir sama dengan hasil eksperimental yang digunakan sebagai pengesahan. Penambahan hidrogen sebanyak 0% - 90% meningkatkan suhu dalam silinder dari 1017 K pada 0% hingga 1200 K pada 90%, ketika nisbah kesetaraan ialah 0.6. Pada 90% penambahan hidrogen, suhu maksimum silinder 1424 K telah diperoleh. Pengurangan tekanan dalam silinder dari 3.200 bar pada 0% hidrogen kepada 2.872 bar telah diperoleh pada 90%. Kenaikan dalam nisbah kesetaraan telah meningkatkan tekanan kepada 3.228 bar pada nisbah kesetaraan 1.4 dan 0% hidrogen. Kadar

pelepasan haba (HRR) meningkat apabila kedua-dua; pecahan mol hidrogen dan nisbah kesetaraan meningkat, dengan 37.98 KJ ketika kadar pelepasan haba maksimum yang diperhatikan pada penambahan 90% hidrogen dan nisbah kesetaraan 1.4. CO meningkat dengan hidrogen dan menurun dengan peningkatan dalam nisbah kesetaraan. Pada 90% hidrogen (nisbah persamaan 0.6), maksimum CO pecahan mol 0.0306 telah diperoleh, manakala minimum 0.0201 diperoleh pada nisbah kesetaraan 1.4. Sebaliknya, pelepasan pecahan mol CO_2 telah menurun dengan peningkatan dalam pecahan mol hidrogen dan telah meningkat dengan peningkatan dalam nisbah kesetaraan. Pelepasan NO_x meningkat dengan peningkatan dalam kedua-dua parameter. Pecahan mol metana tak terbakar meningkat dengan pecahan mol hydrogen, dan menurun dengan peningkatan dalam nisbah kesetaraan. Nisbah pusaran (swirl ratio) pula menurun dengan penurunan dalam kedua-dua parameter, manakala nisbah putaran (tumble ratio) meningkat masing-masing dengan peningkatan dalam kedua-dua parameter. Analisis kontur mengenai kesan penambahan hidrogen terhadap kehilangan fluks haba menunjukkan bahawa sebahagian besar kontur api mengembang di sekitar mangkuk piston dengan peningkatan dalam pecahan mol hidrogen. Penambahan hidrogen meningkatkan nisbah putaran. Julat maksimum halaju ialah 9.72-8.26 m/s dan 6.80-5.35 m/s di dalam kawasan mangkuk piston. Dapatan menunjukkan bahawa, peningkatan hidrogen dalam gas diesel asli meningkatkan ciri pembakaran dan mengurangkan pelepasan pada enjin CI.

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LIST OF SYMBOLS AND ABBREVIATIONS

ASTM	American society for testing and materials
BDC	Bottom dead center
BMEP	Brake mean effective pressure
BSFC	Brake specific fuel consumption
BTE	Brake thermal efficiency
CAD	Crank angle degree
CFD	Computational fluid dynamics
CFR	Cooperative Fuel Research
CHP	Combined heat and power
CI	Compression ignition
CNG	Compression natural gas
CR	Compression ratio
DI	Direct injection
DICI	Direct injection compression ignition
DME	Dimethyl ether
EGT	Exhaust gas temperature (K)
GHG	Greenhouse gases
GT	Gigaton
HCCI	Homogeneous charge compression ignition
HCNG	Hydrogen-natural gas blends
HRR	Heat release rate
IC	Internal combustion
IMEP	Indicated mean effective pressure
LCA	Life Cycle Assessment
LHV	Low heating value
LHV_m	Lower heating value on mass
LHV_v	Lower heating value on volume

LPG	Liquefied biogas
MBDOE	Million barrels per day of oil equivalent
MN	Methane number
PDF	Probability density function
PI	Port injection
PM	Particulate of matter
RFL	Rich flammability limit
rpm	Revolution per minute
SI	Spark ignition
TDC	Top dead center
λ	Excess air ratio
vf	Volume fraction
τ	Sheer stress (pascal)
$\dot{q}$	Heat flux (W/m$^{2)}$
Cμ	Turbulent model constant
ε	Turbulent dissipation rate (m^2/s^3)
μ_t	Turbulent viscosity(m^2/s)
Pr	Turbulent prandtl number
$p(f)$	Probability density function
$(\tau_{ij})_{eff}$	Viscous heating
μ_l	Laminar viscosity $(\mathrm{N/m^2})$
μ_{eff}	Effective thermal conductivity (W/ (m K))
ϕ_i	Instantaneous species mass fraction
$\mathcal{D}$	Effective diffusion coefficient (m^2/s)
ρ	Fluid density $(\mathrm{kg/m^3})$
u	Velocity scaler (m/s)
$\bar{u}_g$	Mesh velocity of moving mesh
nf	Number of face on the control volume
$\bar{A}_j$	Face area vectore (m^2)
δV_j	Volume swept out by the control volume face
$\boldsymbol{\Delta}$t	Time step
ϕ	Equivalence ratio (dimensionless)

α	Mole fraction
CO	Carbon monoxide (mole fraction)
CO_2	Carbone dioxide (mole fraction)
CH_4	Methane (mole fraction)
e	Internal energy$(m^2$kg$)/s^2$
E_a	Effective activation energy (kJ/mol)
f	Force (N)
f	Mixture mass fraction
H	Total enthalpy (energy/mass)
HC	Hydrocarbons
H_2	Hydrogen
H_2O	Water vapour
p	Pressure (bar)
mf	mass fraction
N	Engine speed (rpm)
S	Length of stroke (mm)
S_{ig}	Ignition species source term
NO_x	Nitrogen oxide (mole fraction)
N	Mole number
O_2	Oxygen (mole fraction)
S_p	Pre-exponential coefficient
r	The radius of the crank (mm)
x	Excess air
2DS	2 degree scenario
6DS	6 degree scenario

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CHAPTER 1

INTRODUCTION

1.1 Background of the study

The engine is an integral and most important part of the vehicle that is responsible for the required mechanical power used in the movement of the automobile. Essentially, the mechanical torque is derived from the engine, using the principles of energy conversion. The mechanical power produced by engines is due to the rotational motion of crank shaft which the shaft derive from the movement of the piston between the top dead center (TDC) and bottom dead center (BDC). Equally, the piston movement was on the account of burning the combustion gases (fuel - air mixture) inside the piston-cylinder (combustion chamber). On this ground, the automobile engines are called internal combustion (IC) engines.

Based on combustion mechanism, two principal types of engine are known. The first is the compression ignition (CI), also known as diesel engine. The second is the spark ignition (SI), popularly called the gasoline engine.

The CI engine are used in driving heavy duty machines and in the power generation plants due to the 40% higher efficiency and torque provided when compared to the SI gasoline engines (Jhang *et al*., 2018). The transport sector prefers the CI engines as a choice for Trucks based on the aforementioned advantage. CI engines operate with either the premixed, partial mixed or the non-premixed air-fuel mixing method as induction charge (air-fuel) method. The inducting air is delivered through the suction stroke, while the gaseous and or primary diesel fuels are injected at the end of compression stroke and sequenced to combustion process. When this method is applied, it is called Non-premixed combustion reaction direct injection (Zareei, Rohani & Mahmood, 2018). The introduction of premixed fuels was necessary due to the depletion of conventional hydrocarbon fuels (gasoline and diesel). The advancement in technological innovations, economic challenges, and environmental concerns that the automobile industry has to contend with made the quest for increase in the demand for economical fuels to be on the rise. Compression ignition (CI) direct injection engine is more fuel economical due to high compression ratio obtainable while in operations (Zhao *et al*., 2013b). On the other hand, this engine has disadvantages in contrast with SI engines such as cold start, higher noise, lower speed and high emissions. Despite these aforementioned challenges, the literature has given less attention to assessing the phenomenological features required in exploring alternative fuels. The projected target of such unconventional fuel for the CI engine is to expedite the combustion operations. Partly, there would be reduction in emissions which suggest a substitute for the conventional fuels. By implications, the aforementioned challenges, especially the incessant exploration of the hydrocarbons and depletion of the environment are to be mitigated (Zareei *et al*., 2018).

Automobile engines fueled with natural gas produce less pollution and carbon dioxide (CO_2) in contrast to gasoline-diesel engine. They have higher anti-knock properties which allow them to increase the compression ratio in comparison with a gasoline engine. On the other hand, the compressed natural gas-diesel engine produced more carbon monoxide (CO) and hydrocarbon (HC) emissions than that of normal diesel engines. Thus, low in-cylinder peak pressure and temperature, low engine power and low brake thermal efficiency were some of the limitations of the compressed natural gas-diesel engine. The justifications for these comparatively poor performances was due to the longer ignition delay as well as slow flame propagation speed and burning rate (Khan, Yasmin, & Shakoor, 2015).

The introduction of hydrogen supplements was suggested to be one of the most promising technique to overcome the aforementioned challenges of low performance of the diesel engine. Hydrogen is renewable fuel which could be produced from natural resources; like biomass and fossil fuels (Morais *et al*.,2013). On the benefits of hydrogen as a choice of fuel, it has high diffusiveness. The implication was that a manageable amount of hydrogen injected into the diesel engine was suggested to reduce diesel spray heterogeneity to deliver a uniform combustion mixture (Azimov *et al*., 2011) as high homogeneity would provide an appropriate condition to compete for the combustion reaction.

Also, hydrogen was characterized with fast flame speed, wide flammability range, and low ignition energy. However, the high cost of production of the hydrogen as a fuel was reported to be a challenge. The use of hydrogen as conventional primary fuel in the engine remains a challenge. There are issues of knocking and pre-ignition that hindered the use of hydrogen as a fuel (Park, Kim, & Choi, 2012).

The natural gas-hydrogen fuel mixture could be a practical alternative for fossil fuel due to the high energy efficiency and the total pollutant emission reduction. Natural gas-hydrogen mixture provides an opportunity valid for use in transportation sectors. Also, the desired benefit is not only in combining hydrogen and natural gas, it extends to overcoming the challenge of using either of the alternative fuels as a single alternative. Utilizing natural gas mixed with hydrogen in the internal combustion engine was reported to boost the weak fuel condition during the combustion process (M. Li *et al*., 2020).

Apparently, the future technologies target more of economically viable and environmentally friendly fuel. These made the modelling of Compression Ignition (CI) engine with dual fuel worthwhile and interesting. Previous efforts compared a combination of gaseous fuels like liquefied natural gas / compressed natural gas / hydrogen / synga / biogas along with primary liquid diesel fuel (Khandal, Banapurmath, & Gaitonde, 2018).

The literature is short of phenomenological studies where the theoretical reason for using a tri-fuel model of engines were demonstrated on the Computational Fluid Dynamics (CFD) simulations. The modelling in Zareei *et al*. (2018) concentrated on the dual-fuel engines using compressed natural gas. The theoretical and simulated investigations on dual fuel engines using hydrogen done by Yang *et al*. (2015) lacked the requisite validation to substantiate the claims that hydrogen could be used as an alternative source of fuel in the dual-fuel engine. However, it provided useful information on the potentials of hydrogen fuel. The study was silent on the effect of addition of 0% - 90 % hydrogen to the diesel. The characterization of the emissions were not done with respect to equivalent ration of 0.6-1.4 of HCNG.

The aforementioned studies demonstrated possibilities of the addition of fractions of hydrogen in diesel and gaseous fuels. This suggest that when hydrogen was added, it has effect on the CO, CO_2, and heat release rate (HRR). At the same time, it is difficult to find relevant information on the prediction of combustion and emissions characteristic for CI engines utilizing hydrogen in tri-fuel mode. Suffice to note that bulk of the studies were experimental. This means research on the theoretical and CFD simulations of Methane-hydrogen based on tri-fuel model of compression ignition (CI) engines are scanty. The financial implications, level of accuracy and resource constraints were partly the challenges in experimental studies (Nithyanandan *et al*., 2016).

1.2 Problem statement

The energy industry in recent years has a number of challenges to contend with. First, environmental degradation is alarming due to the continuous increase in demand for energy leading to more exploration of crude oil. The second challenge is the energy security issue which results from the uncontrolled exploitation of the limited reserves of conventional hydrocarbon fuels, like fossil fuel, natural gas, and coal(Yip *et al*., 2019). On the aforementioned grounds, the quest for alternative fuels is increasing more than ever. There are various solutions proposed for diesel engines by many scientists, and the use of gaseous fuels as a supplement to diesel fuel is one of the most important solutions. Efforts by previous studies were limited to the use of compression natural gas (CNG) as an alternative to the transportation sector (Song *et al*., 2017). These proposals were hinged on the availability and cheap price of the CNG. Methane constitute major part of CNG and contain anti-knocking agents, meaning knocking can be avoided by the use of CNG under normal circumstances with higher thermal efficiency at high compression ratio comparatively than that of normal gasoline (Demirbas, 2010). Natural gas volumetric efficiency is lower than liquid fuel, leading to a reduction of power output. While this process can be overcome by directly injected the gaseous fuel (natural gas) into the combustion chamber of the engine during the compression stroke, it still limited to the problem of lacking oxygen concentration during the combustion reaction process. Thus, even with this modification, the natural gas-diesel engine still suffers the low of the thermal efficiency and output power due to a low of a laminar flame speed.

Hydrogen as a supplementary fuel could overcome the problems relevant to natural gas engines. Moreover, it will alter the dependency for conventional fossil fuel. Hydrogen accelerate the combustion flame speed, which offers a wide of range flammability, and supports the low ignition energy. Therefore, hydrogen-enriched compressed natural gas (HCNG) plays an important role for a promising alternative fuel type. The adoption of hydrogen and methane blended with diesel are alternatives targeted at the future and current diesel CI engine technologies. It should be noted that to study this tri-fuel application on CI engine are more practical to be modeled by numerical calculation than experiment in the light of financial and technological constraints.

1.3 Objectives

The chief aim of this study is to investigate the effect of hydrogen enrichment on a dual-fuel direct ignition diesel engine using ANSYS.

Following are the objectives targeted at achieving the aim:

i. To develop a reliable CFD model capable of predicting the key parameters in the combustion process of a DI-diesel engine.
ii. To investigate the effect of hydrogen (0 % - 90 %) addition and equivalence ratio (0.6-1.4) of HCNG blends on the combustion and exhaust emission characteristics.
iii. To investigate the relationship between hydrogen and equivalence ratio variations on the air-fuel dynamic flow characteristics.

1.4 Scope of study

This research focuses on hydrogen-natural gas blends fuel on combustion, emission and air-fuel flow characteristic for direct injection diesel engine. The scope of the research are as follows:

i. The compression ratio of internal combustion engine designed to 15:1. This value is specified for moderate engine operations.
ii. Decomposition sector angle was set at 60^o while three-dimension model was divided into six equal part. Only one part of the model was used throughout the simulation process.
iii. Induction stroke started at 570^o crank angle degree (CAD), while exhaust stroke finished, and emission gas was releases at 833^o CAD.

iv. Gaseous fuels injection started at 721^o CAD while the injection stops at 742^o CAD.

v. Position for the injector in radius coordinates was 0 mm in height and 0 mm for a radius with fuel injection angle set at 70^o.

vi. The operations of the combustion engine were specifically designed to work at 1500 rpm and low load of 20 %.

vii. The swirl number for internal combustion engine (ICE) was used to patch the velocities in the chamber in order to start the simulation at angles other than top dead center (TDC). Here the default value was set at 1.3.

viii. Inducted air temperature and pressure were set at 300 K and 3.2 bar. While the injected fuel velocity was 400 m/s.

ix. Fluent or Chemkin File, CI Engine and Diesel laminar Flamelet Species Model were used as material input, engine type and models respectively.

x. Hydrogen addition varied between (0 – 90%) with each step set at 10% mole fraction. Equivalence ratio varied between (0.6 - 1.4) with each step at 0.2.

xi. Combustion characteristic was demonstrated via crank angle degree.

1.5 Significant and justification of the study

The main significance of this study is to provide a quantitative assessment of a novel operating conditions when blended fuel is used in an IC diesel engine. This was done with the intent of reducing the volume of diesel used in the operations of the engine. The investigation of the effect of addition of hydrogen to enhance the dual-fuel direct injection diesel engine using CFD on Ansys suggest options for the engine designers to consider the blending of the fuel for economic and environmental challenges.

The study on the effect of alternative fuels in the modern engine is relevant to the energy industry as a parameter for justifying the efficiency of other types of fuel in the diesel CI engine. The choice of the DI engine was based on the need to reduce the drop-in power output and un-controlled combustion process. The characteristics measured were suitable with the engine when hydrogen was added to the diesel fuel. While the data expands the combustion engine horizon in contrast to the conventional diesel engine.

The scanty nature of data on the direct injection compression ignition (DICI) engine was a gap that stregthened the novelty of this study. This is because practical data on the techniques deployed in this study lacked the accuracy of numerical studies, to the best of the knowledge of this thesis. This made the computational analyses relevant to the automobile and energy industries.

The dependency on fossil fuels is one of the motivations of this research. The choice of parameters used in assessing the effect of alternative fuel on different outputs of the combustion engine were done to fill the identified gaps in literature. Finally, fossil fuel burnings release greenhouse gases (CO, CO_2) and other pollutants (NO_x, $SO_x$and particulate matter) into the atmosphere and such emissions are increasing day by day.

Hydrogen as a fuel has a promising future in the energy industry. The numerical analysis was done with the intent of promoting green innovations, hence hydrogen was projected as a good alternative source of energy instead of conventional fuels. Hydrogen reacts with oxygen leading to a hypothetical economy which is expected to be used in energy generation for vehicle engine and the electric machine. The hydrogen is a good competitor against fossil fuel usage. Moreover, it is believed to be a sunrise industry that would contribute to reducing energy consumption and emissions, as well as stimulating economic growth.

Using the direct injection techniques when hydrogen is blended with natural gas in the form (H_2+CNG) + Diesel is scanty in literature. From highlighted studies as demonstrated in the synopsis of literature presented in Table 2.3. It is observed that there is no significant information about the un-burnt methane concentration, turbulent kinetic energy, swirl ratio and tumble ratio. Such kind of data plays a vital role in the combustion reaction process and considered as a novelty. The CFD simulation on (H_2+CNG) + Diesel fuel in (CI) engine where the effect of varying proportions of hydrogen alongside the quality of combustion characteristics (in-cylinder temperature, in-cylinder pressure, and Carbone monoxide) and equivalence fuel-air ratio are missing in the previous studies.

1.6 Organization of the thesis

This thesis consists of five chapters. The first chapter covered the research background, problem statement, objectives of the study, scope of the study, significance of the study and organization of the thesis.

Chapter two covered the research literature on internal combustion emission and previous studies related to alternative fuels used in combustion engine, Sources of air pollution such as particles and pollutant gases were also presented. On top of that, the chapter discussed modifications done on fuel injection technique in the engine.

Chapter three described the research methodology in detail. This chapter also offered a CFD approach to give sufficient visualization used in simulating. This chapter extended to creation of an engine model, decomposition technique, meshing process, the boundary conditions used in the simulation modeling, and analysis set-up.

Chapter four analyzed the CFD results, which were discussed using comparable experimental and numerical data from past studies. In addition, this chapter also showed the model validation with an experimental study from the literature before capping it with studies on refinement of meshing sensitivity.

Chapter five concluded the study based on the objectives and in accordance with the results of the study. Valuable recommendations were drawn as the thesis suggested directions for future work.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

The aim of this chapter was to identify the gaps by conducting a thorough assessment of relevant and recent studies on the effect of hydrogen enrichment when used as a dual fuel in the direct ignition diesel engine. The focus was to explore simulations in CFD on Ansys. The chapter commenced by appraising types of fuels used in compression ignition engines. Alternative fuel to be used in compression ignition (CI) engine were documented. The need to define relevant types of alternative fuels used in CI engines and their importance was done is a subsection of this chapter. Further presented were the parameters to be considered in using alternative fuel, Current status of production, impact and future directions on alternative fuels and an appraisal of natural gas as alternative fuel in compression ignition engines was done. The demand for the natural gas as a transportation fuel, combustion of hydrogen within IC engine dual fuel and methods of using hydrogen in injection combustion engine were offered. Other subsection reviewed are effect of hydrogen addition on emission, the carbon dioxide released, and features of carbon monoxide. The chapter was capped with a summary where identified gaps were discussed, and the novelty briefly outlined.

2.2 Fuels used in compression ignition engines

Compression ignition engine operates using vaporized and mixed fuel in appropriate proportional of air before ignition occurs (Swami, Mallikarjuna & Ramesh, 2010). This process is fully controlled by the kinetics of chemical properties. It is key to specify the fuel auto-ignition point for a smooth operation of engine free of misfiring or knocking. Various fuels will result in multi auto-ignition point. Figure 2.1 illustrates the auto-ignition temperature for different fuel at different compression ratio as obtainable in compression ignition engine (Swami *et al*., 2010).

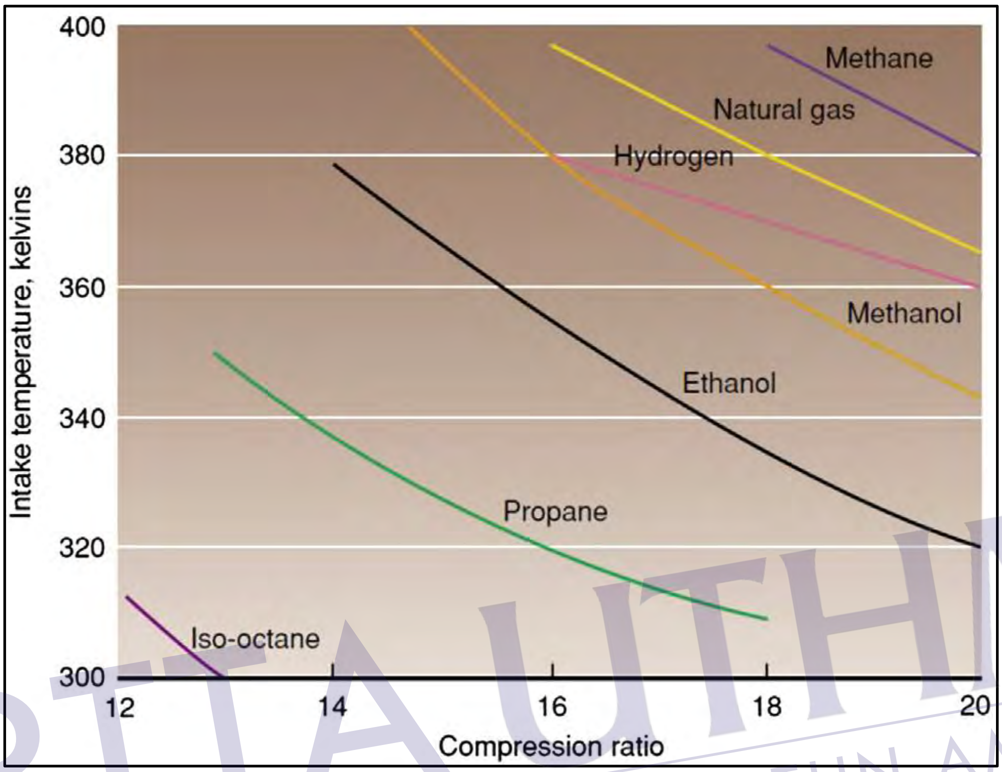

Figure 2.1: The intake temperature versus the difference in pressure ratios required for fuel to operate under homogeneous charge compression ignition(HCCI) mode (Swami *et al*., 2010)

Clearly, methane requires higher intake temperature of 380-400 K and a compression ratio of 18.5-20.0 in order for auto-ignite to occur. It should be noted that hydrogen require 360-380 K and a compression ratio of 16.0-20.0. The implications are that an increase in the number of carbon atoms resulted in decrease in auto-ignition point. The high compression ratio means that the engine was suggested to extract more mechanical energy from the air-fuel mixture as a result of the higher thermal efficiency. Specifically, less fuel would be required at higher compression ratios in addition to the longer expansion cycle, increased mechanical power output and lower exhaust temperature.

From the summary of the properties of fuels that are used in the CI engine presented in Table 2.1, it was obvious that methane has the highest auto-ignition temperature of 923 K. The auto-ignition temperature of hydrogen and diesel are 858 K and 553 K respectively. The implications are that methane spontaneously ignites in a normal atmosphere without an external source of ignition faster than hydrogen and diesel. A comparative breakdown of the conventional diesel fuel alongside hydrogen and natural gas is presented in Table 2.1.

Table 2.1: Diesel properties compared to hydrogen and natural gas (Saravanan, Nagarajan, Sanjay, Dhanasekaran, & Kalaiselvan, 2008)

Properties	Diesel	Hydrogen	Natural gas
Main component	$C_{12}H_{23}$	H_2	Methane CH_4
Auto-ignition temperature (K)	553	858	923
Lower heating value (MJ/kg)	42.5	119.93	50
Density (kg/m^3)	833-881	0.08	0.862
Molecular weight (g/mol)	170	2.016	16.043
Flammability limits in air (Vol%)(LFK-UFL)	0.7-5	4-75	5-15
Flame velocity (m/s)	0.3	2.65-3.25	0.45
Specific velocity (m/s)	0.83	0.091	0.55
Boiling point (k)	453-653	20.2	111.5
Cetane number	40-60	-	-
Octane number	30	130	120
CO2 emission (%)	13.4	0	9.5
Diffusivity in air (cm^2/s)	-	0.61	0.16
Min ignition energy (mj)	-	0.021	0.21

2.3 Alternative fuel for compression ignition engine

Diesel fuel has been described as the conventional fuel for compression ignition engine. The distinct difference between compression ignition (CI) and spark ignition engine is that fuel is directly injected into the cylinder in the case of the CI engine. On top of that, auto-ignition is obtained at high ambient temperature, while the combustion cycle passes from the inlet stroke through the direct compression stroke and exhaust. This is why fuel with auto-ignition ability is required in the operations of compression ignition engines. There are several critical criteria upon which the quality of alternative fuel to be used in place of diesel fuel are measured to make it suitable for compression ignition engines (Varanda, Pinto, & Martins, 2011). These are:

i. Boiling point

ii. Cetane number

iii. Viscosity and narrow density

Cetane number is a strong measure of the characteristics of fuel ignition quality. Also, it is the primary significant factor which gave alternative fuel applicability in compression ignition application. For instance, n-hexadecane has 100 cetane number, which made it easily ignite, while methyl naphthalene has zero cetane number that ascribed it as slow-ignition.

Earlier, Cooperative Fuel Research (CFR) Committee, a single-cylinder standard was used to measuring the cetane number of unknown fuel, before it was later standardized as ASTM D613. The process was to add n-hexadecane for the mixture gradually with different proportions until the same ignition delay of the unknown fuel is obtained. Hence, n-hexadecane proportion considers Cetane number. It has been approved that cetane number may exceed 50 if desired for the purpose of the optimization process in modern applications (Varanda *et al*., 2011).

Figure 2.2 is a representation of a conceptual model that finds application in conventional spray diesel combustion through a quasi-steady period as offered by (Wan *et al*., 2015). It was reported that the process commenced with the spray of liquid fuel before graduating to a point where the mixture of fuel/air in a vaporized phenomenal.

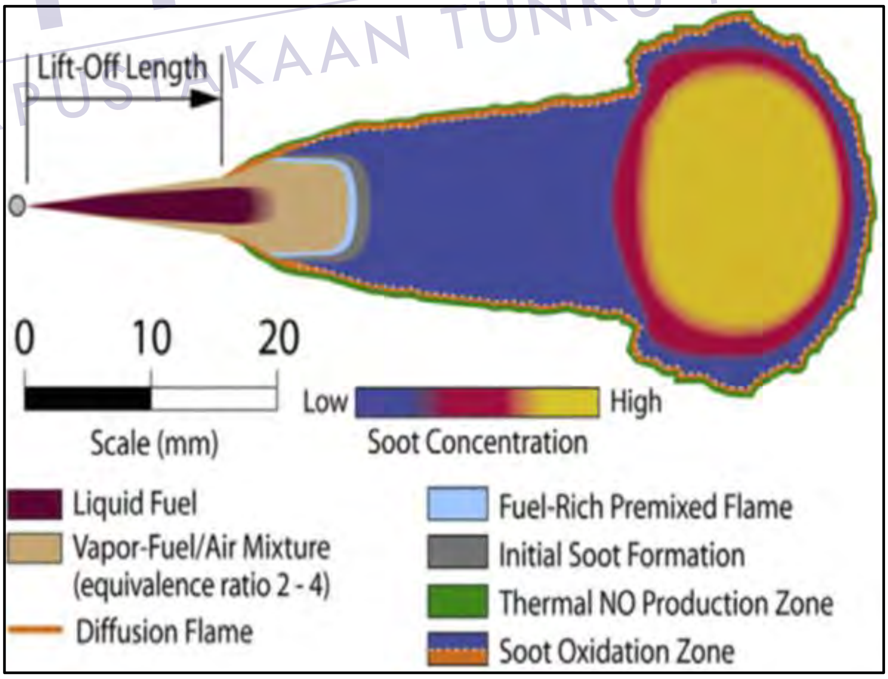

Figure 2.2: Conceptual of conventional diesel combustion process (Wan *et al*., 2015)

The mixture had an equivalent ratio of 2-4 fuel/air. Formation of soot only commenced after a rich premixed flame was obtained. This conceptual combustion process suggests that a blend of diesel and hydrogen was possible before the fuel transformed from the liquid state to the vapor state. The diffusion flame was the third stage of combustion and is a distance away from nozzle downstream.

2.4 Alternative fuels and importance

Alternative fuels characterization could vary from one environment to another. Current research defined alternative fuels as possible replacements to conventional diesel and gasoline fuels. These alternative fuels vary in properties, sources, forms, and methods of manufacturing. For instance, ethanol fuel was considered as a replacement for spark ignition engines. It can be obtained from conventional crude oil or renewable biomass sources. The alternative fuels advanced by Act Policy Energy also covered a large number of non-conventional fuels, as well as alcohol. The alcohols as classified as containing a mixture of gasoline with a ratio of more than 85 %. Natural gas fuel and domestic liquefied natural gas fuels, coal liquid fuels, liquefied petroleum gas, biodiesel, hydrogen (H_2), and significantly petroleum-free fuels were recognized as major security energy and environmentally beneficial.

The importance of alternative fuels usage was ascribed to the following features

i. In pursuit of energy sustainability by extending the use of alternative fuels from renewable sources and reducing fossil fuel energy concerns.
ii. Increased engine efficiency and engine emissions compared to conventional fuels with alternative fuels having higher physical or chemical characteristics.
iii. Relieve the imbalance in the use of traditional petroleum-based fossil fuels.

The pursuit for a stable source of all types of renewable energy is relevant to achieve the desired improvement in the use of alternative sources of energy and reduce the dependence on conventional sources of energy. It should be noted that the rise in energy demands is a challenge to the limited amount of fossil fuels available (Salvi and Panwar, 2013).

The US Information Energy Administration, 2013 in combination with the outlook for security energy (sustainability energy) and the focus on greenhouse gases

(GHG) reduction over the next 50 years, had encouraged an increase in the use of renewable biofuels. The report put forward major challenges in the use of fossil fuels as the emissions of carbon dioxide. Moreover, human activities generate approximately 30 billion ton of carbon dioxide per year (Y. F. *et al* ., 2014). The obvious challenges on the environment, health and energy economy are sufficient reasons for adopting alternative sources of fuel. The reports and policy directions are relevant in showcasing the opportunities, but the implementation must commence by simulations, hence technology adoption by the industries must be based on scientific proofs.

The full Life Cycle Assessment (LCA) is a method of comparing the effects of different traditional fuels and biofuels on greenhouse gases (GHG). The analysis takes into account the concern of greenhouse gas emissions from production, storage, and transport, in addition to emissions from the use of vehicles. The renewable biofuels were suggested to be a way of reducing the life cycle of carbon dioxide (CO_2) emission based on the LCA. However, biofuels usage represents about 4% of total international transport fuel as reported by (Abdalla *et al*., 2018). The products of used biofuels from vegetable oil formed using biomass as feedstock and energy sourced from ethanol and corn were on the suggested list of fuels that support the reduction in CO_2 emission. With this, emissions will be reduced to about half of the conventional fuel consumption (Streimikiene *et al*., 2013). The demand for various types of fuel by the transportation sector is presented in Figure 2.3.

Figure 2.3 showed that recently, request for energy in the transport sector is continuously increasing, fuel-to-fuel ratio is also expected to increase from the Energy Outlook (Kalghatgi, 2015). The implications, with specific emphasis on diesel used in the compression ignition (CI) diesel engines, are that the consistent increase in the Million Barrels per Day of Oil Equivalent (MBDOE) means increase in the emission of CO_2 and consistent pollution in addition to environmental degradation. The concept of introduction of hydrogen to the diesel was aimed at reducing this consistent increase in demand. Suffice to note that scientific investigations are better appreciated with models than experimental due to the financial constraint in demonstration of the blending of diesel with hydrogen. This is where CFD comes handy.

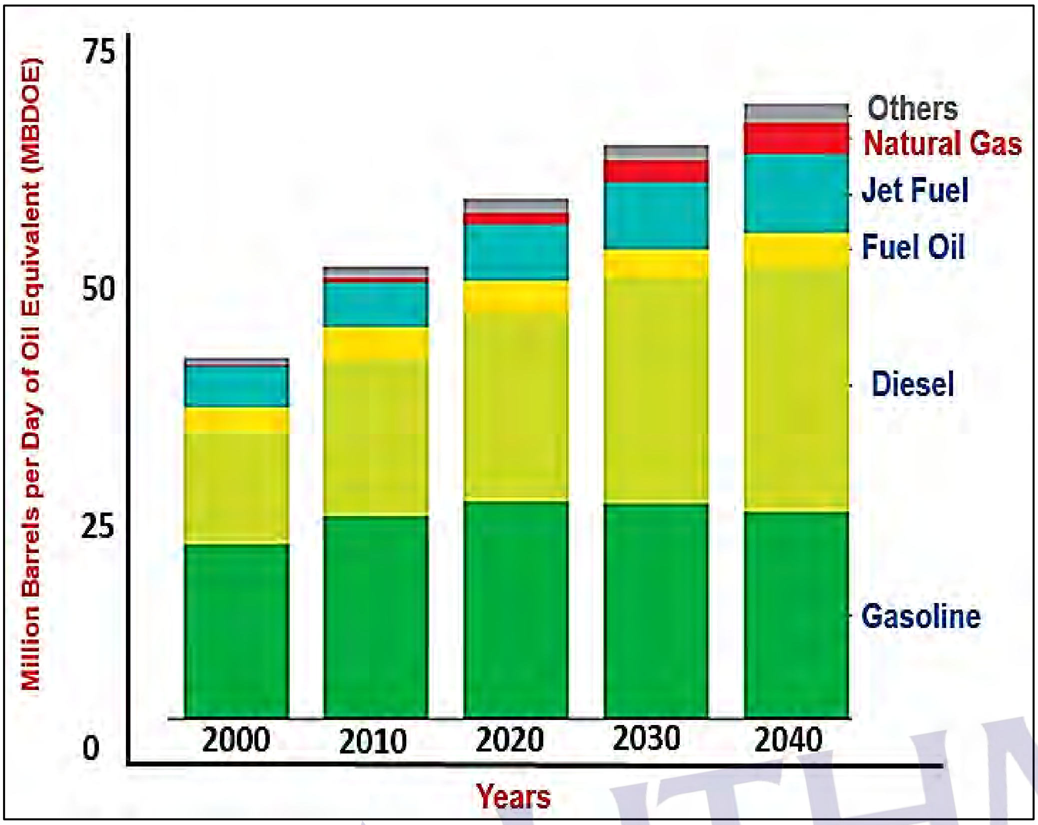

Figure 2.3: Global transport demand for fuel (Kalghatgi, 2015)

More on the effect of demand for diesel and exhaust emissions is presented in Figure 2.4. The 2 degree scenario (2DS) and 6 degree scenario (6DS) showed the cumulative contributions of fuels to the emission and relationship with CO_2. From the technique viewpoint, an increase in the acceptability of biofuels, renewable or alternative fuels suggests an improved performance of the engine and characteristics of emissions.

The balancing between harmful emissions and fuel efficiency like in non-combustible hydrocarbons (HC), NO_x, carbon monoxide and particulate of matter (PM) has always been considered as vital issues in direct ignition, combustion diesel engine related studies. More so, fuel combustion is specified by fuel-air interface. Distinctively, the use of alternative fuels was suggested to deliver better characteristics when used directly in combustion engine.

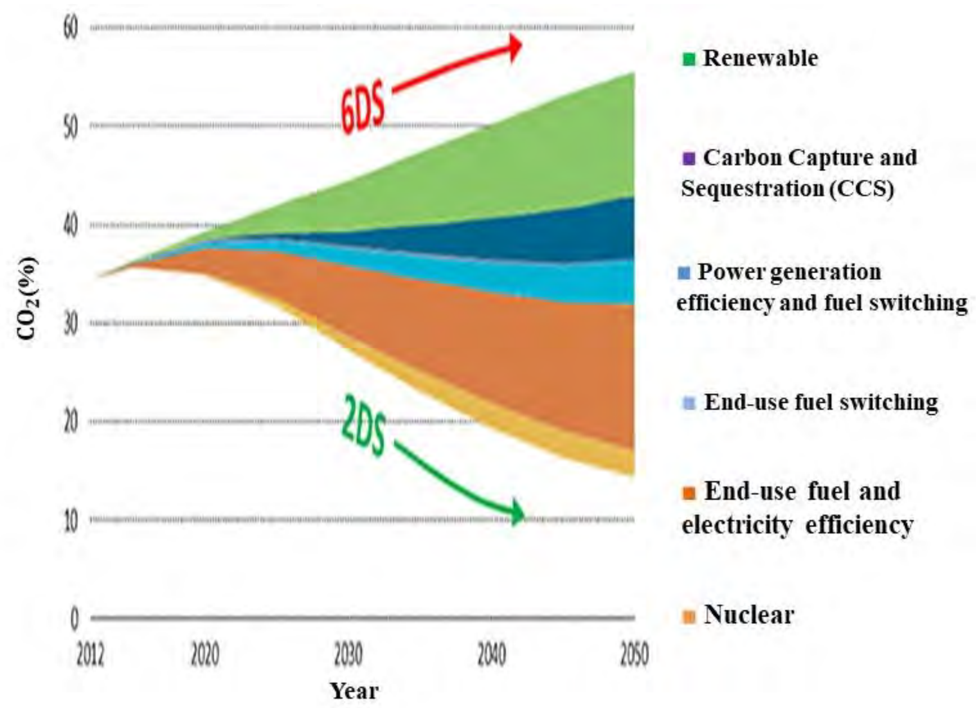

Figure 2.4: Reduction in vehicle exhaust emissions the 6DS and 2DS transmission (Wang *et al*., 2014).

The figure showed that alternative fuels are actually sought for in the operations of internal combustion engines to maximize their acceptability and potentials globally. Energy demand from the global transportation industry is predicted to grow at an annual rate of 1.2% to 1.4%(Kalghatgi, 2015). More efficient vehicle would emerge where low carbon fuels would be used before the end of 2050. Moreover, unstable increase in demand for fossil fuel products could be a source of concern. The ratio of diesel and other medium distillates to gasoline is expected to rise from the current 1.5 gigaton(GT) to about 2.4 GT (Kalghatgi, 2015). From the foregoing, some considerations worthy of assessing for the adoption of alternative fuels for SI and CI engines are summarized in the following point:

i. Properties of combustion are required to be analyzed (chemical properties such as octane and cetane number)
ii. Physical properties (spraying or burning due to combustion, engine operation over a large temperature)
iii. Low-calorie value (LHV)
iv. Compliance (including approvals and vehicle manufacturers' fees)

Apparently, the simulation of the chemical properties is prioritized because subsequent parameters and procedures are dependent on the knowledge of the properties. The findings of Yang *et al*., (2015) had justified the quest for scientific evidence and experimental as basis for consideration of novel fuel blending technologies. Unfortunately, the study failed to establish a basis for the effect of addition of hydrogen beyond the 6%, thereby limiting the dependability of such findings.

2.5 Current status of production, impact and future vision

Figure 2.5 illustrates and summarizes all pathways available for liquid fuel production and certain gaseous fuels from biomass and fossil resources (Masum *et al*., 2013). Currently, most types of transportation engine fuels are derived from crude oil with oil refining technology (Lata *et al*., 2012).

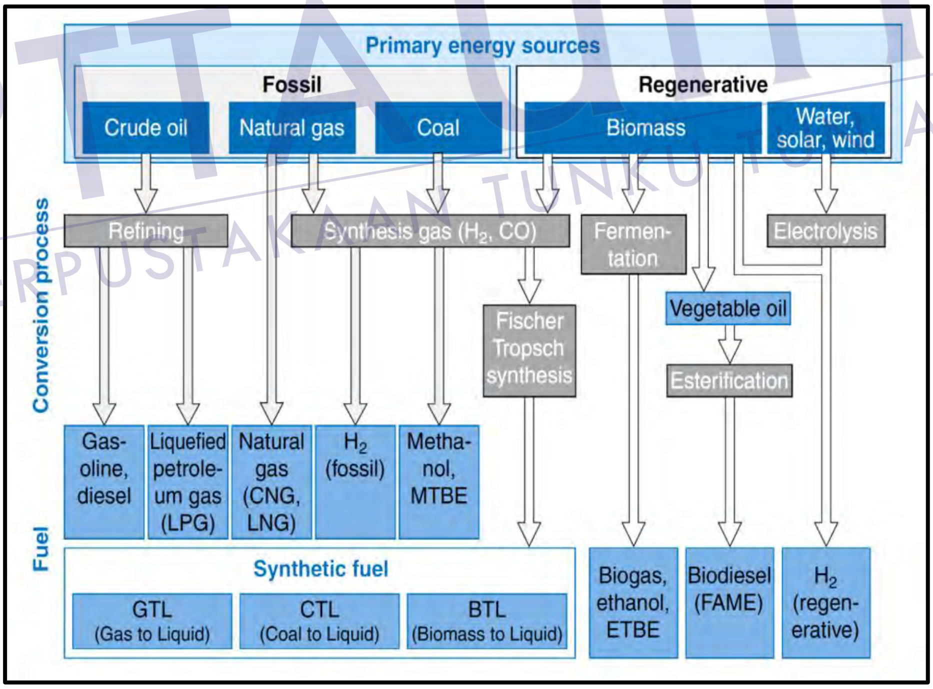

Figure 2.5: Fossil fuels manufacturing and regeneration (Masum *et al*., 2013)

There has been a gradual increase in the sourcing of non-traditional oils like oil shale and oil of sands produced from rock gas. Artificial liquid fuel can be produced with similar properties of oil-derived from the process of gasification of any hydrocarbon feedstock or coal. Some familiar alternative fuels, like ethanol (bioethanol) and biodiesel that were advanced, show sensibility with compounds of ignition in a combustion engine, this average product can also achieve moderate to low emissions of moderate gases. However, Iliev (2015) reported that ethanol has chemical and physical properties comparable to the gasoline, hence more appropriate for SI engines. A reduction in Carbon monoxide (CO) and break power corresponded with increase in ethanol.

Technological advancements have supported the production of second biofuels generation from the traditional first biofuels generation. The target was to increase the efficiency in the production and to encourage the usage of non-edible biomass. The use of food sources will cause food prices to rise and has been widely criticized in the past. Nurusal (2015) had reported that 90% of the palm oil produced is used for food and the remaining 10% for non-food consumption. The biofuel was suggested to deliver higher ignition quality in CI engine due to the higher level of molecular saturation and lower number of double bonds in the molecules. Figure 2.6 shows that compression natural gas and liquid pressure gas compatibility with the current distribution of infrastructure is higher than derived by compressed natural gas (CNG) examples include dimethyl ether (DME) and H_2. These kinds of fuel were suggested to be certified in physical and chemical characterizations for applications in engines with some modifications. Recently, attention in CNG has continued to be on the increase as an alternative fuel because of the availability of shale gas reserves. The proportion of natural gas reserves to production (R / P) was 54 ±2 as at 2015. At the same time, the reserve and production of crude oil (R / P) was about 54 ±2 (Hansen et al, 2005). The implication of this was that the natural gas was suggested to replace crude oil with sufficient time and technology.

Figure 2.6 shows that the proportion of shale gas in total natural gas production in the United States rose from 1% in 2000 to 40% in 2012. The trend was projected to be progressive, with expected rise to 53 % in 2040 (U.S. Energy Information Administration, 2014). The production of shale gas was aimed at delivering a relatively stable price for the natural gas in the energy market. The recent fluctuations in prices of oil were linked to the production of shale gas. The report by Bae and Kim (2017) was clear that the CI engines are potential beneficiaries of the shale gas as fuel. However, the report provided a good opportunity for further exploration, but the ratio, optimum characterization and a CFD model required to adequately predict the proportions of diesel to hydrogen were not considered.

Fuel	Energy density	Production cost with oil at USD 100 / bbl	Distribution infrastructure	Current production and retail availability for vehicles	Compatibility with existing ICE vehicles	Typical GHG emissions	Feedstock	Process
Gasoline	H	Mod	Comp	Comp	Comp	High	Oil from both conventional sources and non-conventional sources, such as heavy crudes and tar sands	Refining
Distillate	H	Mod	Comp	Comp	Comp	High		
Jet fuel	H	Mod	Comp	Comp	Comp	High		
CTL diesel	H	HMod	Cpt	VL	Comp	VH	NG, coal	Gasification / FT
GTL diesel	H	HMod	Cpt	VL	Comp	H		
Grain ethanol	M	HMod	Par	LMod	Par	HMod	Grain crops	Saccharification and distillation
Cane ethanol	M	LMod	Pal	LMod	Par	Low	Sugar crops (cane)	Distillation
Advanced lingo-cellulosic ethanol	M	H	Par	None	Par	Low	-	-
Oil-seed biodiesel	H	HMod	Par	LMod	Par	Mod	Oil-seed crops	Esterification, hydrogenation
Advanced BTL diesel	H	H	Cpt	None	Comp	Low		
CNG	L	LMod	Par	VL	RC	HMod	Natural gas	Gasification / FT
LPG	L	LMod	Par	VL	RC	HMod		
Methanol from NG	L	Mod	VL	VL	RC	HMod	Natural gas	
DME from NG	M	Mod	VL	VL	RC	HMod		
H_2 from fossil sources	L	Mod	VL	VL	RC	HMod	Natural gas	Reforming, compression
H_2 from renewable sources	L	H	VL	None	RC	VL		

Acronyms:
H: high; M: medium; L: low; VH: very high; VL: very low;
Mod: moderate; LMod: low-moderate; HMod: moderate high;
Par: partial; WS: widespread; RC: requires conversion; Cpt: compatible with existing; Comp: complete
Notes: Table classifications are indicative, based on current characteristics and estimates, and apply only to near-term. There may be situations and regions in which these classifications do not apply.

Figure 2.6: Compression natural gas and liquid pressure gas compatibility (U.S. Energy Information Administration, 2014)

2.6 Natural gas as alternative fuel in compression ignition engines

The report on the use of natural gas as a single alternative fuel for CI engines was not favorable in terms of the characteristics. Instead, it should be used within the dual fuel mode engines where pilot liquid fuel ignites the natural gas as well as air mixture.

Lounici *et al*. (2014) conducted an experimental study in order to investigate the possibilities of using natural gas as a supplement in dual fuel mode of a conventional compression ignition engine. Natural gas within dual gas was inducted through individual stream then merged with the intake air and finally compressed such as conventional compression ignition engine. Due to the high-octane number of natural gas-air mixture, the blend could not auto-ignite. Inject drops of liquid at the end of the compression stroke initiate ignition that was required for combust mixture.

Imran *et al*. (2014) conducted an experimental study in order to investigate natural gas port injection. They reported that natural gas mixed with air and passed through a stroke of compression ignition to the end. Similarly, it was reported that methane had a low cetane number in contrast to air. On another hand, methane had highest specific ratio than air. The low cetane number was the justification for the cause of prolonged ignition delay period. The same reason resulted in poor combustion characteristics and a barrier in ignition process. To solve methane ignition issue, various strategies had been used, one of these provide fuel with high cetane number behavior as ignition source. The seven engine speeds and eight diferent load settings were not sufficient in justifying the efficiency of the engine. Beside, the manifold was used in introducing the natural gas and hydrogen was not used as a blend.

Natural gas based dual fuel recorded highest peak pressure in the study conducted by(Patel & Patel, 2017). The experimental study reported that double ignition delay was the challenge of natural gas based dual fuel. The first ignition delay was associated with the pilot fuel ignition, while the second delay was associated with ignition of natural gas-air mixture. It has been stated that pilot fuel based dual fuel has a long ignition delay in comparison with pilot fuel with particular features of single fueling operation. Some studies reported that natural gas based on dual fuel resulted in a reduction in smoke and particulate matter emission which were not detectable.

Generally, low PM emission level was attributed to low Carbone content concentrations level and high hydrogen to Carbone ratio. Induction technique plays a vital role in reducing PM account, while natural gas induced into the intake manifold port has high chances of mixing with air for a long time. This resulted in promotion of homogenously mixture properties (Santoso *et al*., 2013).

The 21.4 liter/minute, 36.2 liter/minute, and 49.6 liter/minute flow rates of hydrogen used in the research by (Santoso *et al*.,2013). were not sufficient as an established proof of the adoption of hydrogen fuel. Three parameters (specific energy consumption, indicated efficiency, and cylinder pressure) were investigated which were at low load. The hydrogen enrichment reduced the cylinder peak pressure and the engine efficiency, but the study was a deficit in obtaining cylinder peak pressures that were under predicted by the simulation. The claim that detailed input data for the hydrogen fuel affected the result was not substantiated by the validation. There are uncovered concerns like the equivalence ration of 0.6-1.4 of HCNG and the effect of hydrogen on the air-fuel dynamic flow characteristics in (Santoso *et al*., 2013).

2.6.1 Demand for natural gas as fuel

Natural gas has been considered as one of most important energy resources which currently ranked 20% on the list of world primary consumption (Imran et al., 2015). Figure 2.7 shows the global primary energy demand from 2000 to 2030.It could be observed that the demand for natural gas will exceed that of coal. It will also constitute about 25% of the total energy demand by 2030. A projection for the future energy shows that natural gas is the fastest growing source of energy demand and the future of its consumption has been forecasted to double between 2000 and 2030 (U.S. Energy Information Administration, 2014).

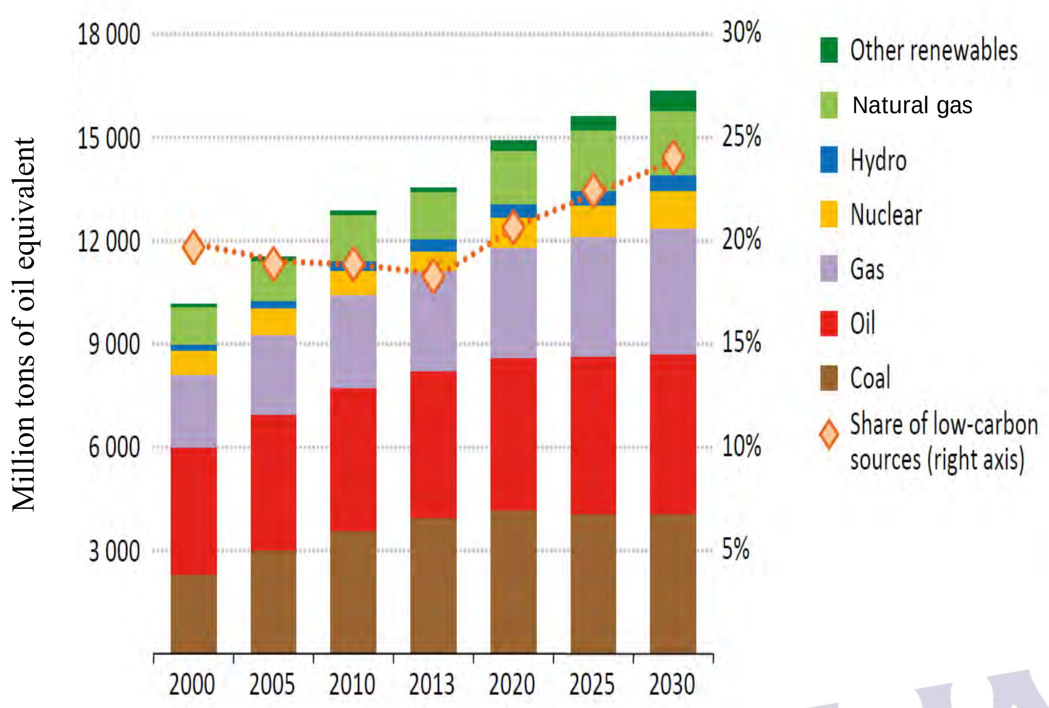

Figure 2.7: Global primary energy demand (Imran *et al*., 2015)

2.6.2 Methane specification

Natural gas is considered a mixture of numerous gases with methane as majority, depending on the source of production, the gases content will differ by concentration. A percentage of 99% represent methane occupation of total content (Akansu *et al* ., 2004). Other hydrocarbon constituents like propane, ethane and butane are in traces as hydrocarbon which could not be included as a content in the natural gas composition. In addition, inert gases such as carbon dioxide, helium, and nitrogen were observed as part of the natural gas (Akansu *et al*., 2004).

Due to environment and economic issues, natural gas has been considered an alternative fuel for combustion engine (De & Panua, 2014). The availability of methane composition, compression natural gas was considered among the cleanest and very important fuel for engine applications. Methane fuel was attributed to slowing of flame propagation which in this respect was responsible for poor combustion capability through lean burning condition. In this regard, natural gas still has some challenges requiring further scientific investigations before it could be considered as an alternative fuel for internal combustion engine.

Properties such as low thermal efficiency, poor lean burning capability, and cycle-by-cycle variation which caused a drop in engine output power and high fuel consumption rate were part of the challenges of using compressed natural gas (CNG). At lean burning condition CNG emits a little amount of exhaust emission.

The advantages of CNG in contrasted of petrol fuel are outlined in the following points;

i. CNG has high octane number so that engine could operate smoothly at high compression ratio and without knocking.

ii. CNG has high capability to blend a unique mixture leading to increase in combustion quality.

iii. CNG has lower flame laminar speed which results in increased durability.

iv. Originally CNG structure constitute methane with helium, propane, nitrogen, and hydrogen and vapor water as traces.

The high-octane number of about 130 was the cause of high methane in CNG, this was responsible for the high persisting to knocking phenomena. Since compression ignition operates at a high compression ratio, it therefore, needs a fuel that has high resistance to knocking phenomena. Accordingly, the high octane number associated with CNG made it suitable as fuel for a compression ignition engine (Talibi et al., 2017). CNG auto-ignition temperature is about 1087 K. Whereas at the top dead center the air temperature is about 800 K. This makes it suitable to be used as fuel in the engine.

When the engine was operating at high compression ratio, CNG as fuel in the engine delivered smooth and high-quality combustion due to the high-octane number of 130. However, in order to setup CNG within conventional engine, minor modification could be required. The unique property of CNG is the possibility of working with a wide range of combustion, attainable at low consumption of fuel and little NO_xemission. This fact stimulated the need for practical investigation of combustion process and emission characteristic in spark – ignition engine fueled by gasoline and CNG (Waller *et al*., 2014).

2.6.3 Methane and diesel in direct injection engine

The process of introducing the methane and diesel for the direct injection engine done sequentially. The technique includes the injection of the natural gas and pilot diesel fuel directly and sequentially into the cylinder and specifically the combustion chamber. Pilot diesel is first injected, followed by natural gas. Mixing occurs at some degree of crank angle and later injected at the compression stroke end (just about the TDC). During the process, the pilot diesel would be auto ignited, based on the conventional diesel engine principles. Comparison between conventional diesel and direct injection for compressed methane engines is summarized in the following points.

i. With conventional diesel injector, injection fuel accrues before compression stroke end by few crank angles, with temperature of the air inside cylinder at about 750-900 K. The pilot diesel fuel passing through nozzle orifices will be atomized, owing to high pressure and temperature inside the cylinder, the vaporized fuel which mix with air auto-ignites (after injection by 2ms)(Fan *et al*., 2018)

ii. In the case of the direct injector operating principles. The methane is injected directly into core of the diesel engine late through the cycle. But self –ignition would not occur at (900-1000 K) which is in-cylinder temperature at the end of compression stroke. Phenomenologically, an improved in-cylinder temperature supports the auto-ignition of the natural gas by increasing the engine compression ratio. The theoretical basis was reasonable but lack practical possibility. Since it was not implementable to get high in-cylinder temperature due to the strength limitation and mechanical stress of the engine. Alternative solution was to use pilot diesel to facilitate the ignition of the methane injected into the engine. This method was suggested to provide stable ignition(Chen *et al*., 2019).

Methane and pilot diesel fuel direct injection is demonstrated in Figure 2.8. Observable here is the jet plumes pattern and injection angles (in both vertical and horizontal planes). Ignition delay plays a vital role in understanding combustion sequences. This sequence could be defined as the time interval enclosed between the

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